

REPORT DOCUMENTATION PAGE			Form Approved OMB No. 0704-0188	
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1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE 4/4/90	3. REPORT TYPE AND DATES COVERED Final Report (11/1/86 - 10/31/89)		
4. TITLE AND SUBTITLE Final Report for Grant "Theoretical Studies of Time-of-Flight and Atom and Molecular Surface Collision"		5. FUNDING NUMBERS 61102F 2303/A3		
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7. PERFORMING ORGANIZATION NAME University of Washington Dept of Chemistry, BG-10 Seattle, WA 98195				
8. PERFORMING ORGANIZATION REPORT NUMBER		9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) AFOSR/NC Bolling AFB Washington, DC 20332-6448		
10. SPONSORING / MONITORING AGENCY REPORT NUMBER AFOSR-87-0075		11. SUPPLEMENTARY NOTES		
12a. DISTRIBUTION / AVAILABILITY STATEMENT Approved for public release; distribution is unlimited		12b. DISTRIBUTION CODE		
13. ABSTRACT (Maximum 200 words) One major project has been finished and two important projects were well underway when funds were cut off. <b>I.</b> The finished work, dealing with cross sections for scattering from defects on surfaces, will be a classic work, since the definition of the cross section had not been done properly before. <b>II.</b> The second project has to do with trapping and sticking coefficients in low and medium energy collisions of atoms and molecules with surfaces. <b>Our</b> aim is to lay to rest the long standing debate regarding the low energy asymptotic limit of sticking coefficients: is it 0? or 1? <b>III.</b> A student was looking at improvements to the wavepacket code for atom surface collisions. He also had started a project involving atom scattering with a vibrating adatom on a surface. <b>IV.</b> Another unfinished project is inspired by some data that Tom Engel has generated on scattering of helium from stepped surfaces. He sees, at certain angles aimed into the steps, a scattering in non-Bragg directions, even though there is supposedly little or no disorder. The scattering is at half the momentum transfer of the perfect surface and rather broad, suggesting that perhaps steps of twice the usual length are involved.				
14. SUBJECT TERMS		15. NUMBER OF PAGES 3		16. PRICE CODE
17. SECURITY CLASSIFICATION OF REPORT Unclassified	18. SECURITY CLASSIFICATION OF THIS PAGE Unclassified	19. SECURITY CLASSIFICATION OF ABSTRACT Unclassified	20. LIMITATION OF ABSTRACT UL (Unlimited) SAR (Same as Report)	

## Final Project Summary- Eric. J. Heller

We have developed the theory for cross sections for scattering from defects on corrugated surfaces. Just as in the gas phase, one needs to have a definition of what is meant by the "size" of an object, as measured by collisions. The history of this problem has been fraught with mistakes and misconceptions. The correct definition of such cross sections had not been given before. The theory allows a rigorous measurement of the "size" of a defect or of an adsorbate, etc, on a surface. The optical theorem was derived for the case of scattering from a corrugated surface. It is interesting in that the "forward" scattering of the textbook optical theorem becomes the Bragg scattering. The optical theorem again is the flux conserving law which states that flux lost from the Bragg directions is recovered as diffuse scattering in between.

The theory was applied successfully to the system CO on Pt (111), resolving a long standing controversy on whether CO is much "larger" on a surface than in the gas phase. In fact it is only slightly "larger".

Another project has examines trapping and sticking coefficients in low and medium energy collisions of atoms and molecules with surfaces. Our aim has been to lay to rest the long standing debate regarding the low energy asymptotic limit of sticking coefficients: Is it 0? or 1? This project is about 2/3 completed. The issue of sticking at low temperatures and low collision energy has important space physics applications.

Finally, the wavepacket code for atom surface collisions has been significantly enhanced. Faster means of propagation have been developed. We have begun a project involving atom scattering with a vibrating adatom on a surface.

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## Final Report- Eric. J. Heller

One major project has been finished and two important projects were well underway when funds were cut off.

- I. The finished work, dealing with **cross sections for scattering from defects on surfaces**, will be a classic work, since the definition of the cross section had not been done properly before. Anyone wishing to measure the "size" of a defect or of an adsorbate, etc, on a surface will need the formula and methods developed by us. Coworkers: Daniel Huber, postdoc; Han Xu, student.

### *Details:*

The first paper is finished, dealing with (1) the definition of the cross section of a defect on a surface, and (2) specifically the system CO on Pt (111). We could have easily split this into two papers, namely a theory paper and an application paper, and this would have surely helped us with those who count papers and don't assess them for quality and impact.

*No one has ever defined the cross section for surface defect scattering on a corrugated surface before; we believe our work to be a real landmark in this respect. Just as in the gas phase, we need to have a definition of what is meant by the "size" of an object. The history of this problem has already been fraught with misconceptions.*

The calculations of CO on Pt (111) have been successful, and compare well with the experiments. Semiclassical wavepackets have been used to perform the calculations. More details are to be found in the manuscript.

- II. The second project has to do with trapping and **sticking coefficients in low and medium energy collisions of atoms and molecules with surfaces**. Our aim is to lay to rest the long standing debate regarding the low energy asymptotic limit of sticking coefficients: Is it 0? or 1? This project was about 2/3 completed, when funding was cut off. Coworker: John Frederick, Postdoc.

### *Details:*

The issue of sticking at low temperatures and low collision energy has important space physics applications. Moreover, it has important experimental consequences since atoms can be dropped onto surfaces at very low velocity using laser atom traps with gravity as the accelerating agent.

- III. A student, Colin Wright (grad student, physics) was looking at **improvements to the wavepacket code** for atom surface collisions. He also had started a project involving atom scattering with a vibrating adatom on a surface. When his funding AFOSR was cut off, he left graduate school. The project is now in limbo.
- IV. Another unfinished project is inspired by some data that Tom Engel has generated on **scattering of Helium from stepped surfaces**. He sees, at certain angles aimed into the steps, a scattering in non-Bragg directions, even though there is supposedly little or no disorder. The scattering is at half the momentum transfer of the perfect surface and rather broad, suggesting that perhaps steps of twice the usual length are involved.
  - 1. H. Xu, D.P. Huber and E.J. Heller, "Cross Section and Optical Theorem for Defects on a Corrugated Surface," *J. Chem. Phys.*, **89**, 2550 (1988)

FINANCIAL STATUS REPORT				U.S. AIR FORCE				AFOSR-87-0075				FEDERAL AGENCY OR OFFICE IDENTIFYING PROJECT				DATE OF REPORT			
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